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13. ABSTRACT (Maximum 200 Words) Experimental studies on several Sm-Co systems have been carried out in search of improved properties of high-temperature hard-magnet materials. An important result, a record coercivity of 12.3 kOe at 500°C, has been achieved in a Sm-Co-Cu-Ti alloy with a relatively simple annealing procedure. Model calculations are able to explain the increase and then decrease of H_c with temperature. Several other Sm-Co-X and rare earth-Co alloys have been studied through mechanical-milling methods. Self-consistent electronic structure calculations have been made on Nd-Fe compounds and the effects of lattice expansion through hydriding determined.				
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AFOSR Final Technical Report

2. Objectives

The objectives remain as stated in the original proposal.

3. Status of Effort

A significant advance has been made in preparing a Sm-Co-Cu-Ti with excellent hard properties at high temperature ($H_c = 12.3$ kOe at 500°C). This has been reported by "High-Tech Materials Alert," John Wiley & Sons, on May 5, 2000. The significance of the work is that a simple, four-element alloy without Zr substitution can achieve significant properties including a positive change of coercivity with increasing temperature. Additional experimental and theoretical research has given an understanding of exchange-coupled hard magnet materials and their dependence on nanostructure.

4. Accomplishments/New Findings/Highlights

4.1 Electronic Structure Studies of RE-TM Compounds

First-principle studies have been carried out to study the magnetovolume effect in $\text{Nd}_3\text{Fe}_{17}$. Hydrogenation of this compound ($\text{Nd}_3\text{Fe}_{17}\text{H}_{16}$) produces 14.4% volume expansion and increases its Curie temperature and magnetization by 14% and 20% respectively. Calculated results are in good agreement with the experimental data. Calculations also show that 6-7 H atoms per formula unit should produce the maximum increase in T_c of $\sim 34\%$ in this compound.

4.2 Sm-Co-Cu-Ti High-Temperature Permanent Magnets

A class of promising permanent-magnet materials with appreciable high-temperature coercivities has been investigated and an H_c of 12.3 kOe at 500°C obtained. The Sm-Co-Cu-Ti magnets are prepared by arc-melting and require a suitable heat treatment. Magnetization measurements as a function of temperature and x-ray diffraction patterns indicate that the samples are two-phase mixtures of 2:17 and 1:5 structures. Depending on heat treatment and composition, some of the magnets exhibit a positive temperature coefficient of coercivity. The promising high-temperature behavior of the coercivity is ascribed to the temperature dependence of the domain-wall energy, which affects the curvature of the walls and the pinning behavior.

4.3 Mechanically Alloyed High-Temperature Magnets

High temperature magnetic properties of RCO_5 ($\text{R}=\text{Sm}$ and Y) have been studied. The samples were prepared by mechanical alloying and subsequent annealing. X-ray diffraction analysis show that the annealed materials have the hexagonal CaCu_5 structure with 2:17 (or 1:7) regions as a minor phase. Our experimental work shows that SmCo_5 and YCo_5 have nearly the same properties

at temperatures above about 500 °C. This fact, which may lead to the development of rare-earth free high-temperature permanent magnets with moderate energy products, is explained by the negligibly small rare-earth anisotropy contribution at high temperatures.

4.4 Exchange-Coupled Magnets

Much experimental and theoretical work has been done on the magnetism of exchange-coupled nanostructures. First, we have shown in much detail how grain boundaries affect the magnetic behavior of nanostructures. The intergranular interactions, realized by the grain boundaries, is accompanied by a very complicated spin structure in the grains. Second, we have investigated how this intergranular exchange affects the hysteretic behavior of the nanostructures. Depending on grain-boundary structure and grain-size, the calculations yield a variety of cooperative effects which enhance the remanence and make the hysteresis loop more rectangular but also reduce the coercivity. In the weak-coupling regime, the magnetization reversal is determined by non-cooperative localization effects.

5. Personnel Supported and Associated with Project

Faculty: Professors David J. Sellmyer, Sitaram S. Jaswal, Diandra Leslie-Pelecky, Yi Liu, Ralph Skomski, Renat Sabiryanov; Postdoctoral Research Associate: Imaddin A. Al-Omari; Graduate Research Assistants: Jian Zhou and Michael Leonard.

6. AFOSR Publications

Twenty publications have resulted from this grant and another five are accepted for publication.